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Synthesis, structural characterization, DFT studies, hirschfel surface analysis, and molecular docking studies of a Cu(II) complex derived from salicylaldehyde

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ABSTRACT

A novel Cu(II) complex, designated as $[(Cu)_3(Saly)_3]$, has been synthesized and studied using a variety of physiochemical methods, including elemental analysis, UV–Vis, and FT-IR spectroscopy. In order to further investigate the structure of the complex, single crystal X-ray crystallography has also been used, which reveals that the crystal exits in an orthorhombic system with the structural parameters a = 5.2212(4) Å, b = 10.5554(10) Å, c = 21.859(2) Å and Z = 4. The antimicrobial activity of the studied complex is carried out, suggesting it to be strong antimicrobial agent. For in silico studies, molecular docking simulations were performed on the crystal structure of target protein (PDB ID) 1DTD, 3FVU, and 4UXU in order to assess the ability of the investigated complex to attach to these target macromolecules.

1. Introduction

Inorganic chemistry covers a wide range of topics, one of which is the study of the structural investigations of coordination compounds [1]. Coordination of ligands to metal ions may result in the formation of novel compounds with desired properties by improving the biological capabilities of the ligand [1]. Over the years, Salicylaldehyde (saloH) and its derivatives, abbreviated as X-saloH, have been demonstrated to robustly coordinate with metal ions due to their chelating sites and to adopt a range of geometries and coordination modes [2–5]. However, the most prevalent binding site is bidentate chelation through both the carbonyl and phenolato oxygen atoms, but monodentate coordination mode through the deprotonated phenolato oxygen atom also occurs [5]. In addition, the coordination of these ligands to metal ions can result in extended π–stacking systems enabling the metal complexes to interact with biomolecules such as DNA and RNA [1,6]. Substituted salicylaldehydes (X-saloH) have been reported to have potential biological applications such as antibacterial and antioxidant activity [7–9], which enhance with the insertion of different groups on the benzene ring [5,8]. Furthermore, metal complexes may prove to be particularly valuable in the process of developing novel agents for therapeutic applications due to their unique physicochemical properties [10,11]. In addition to the medicinal properties of the metal ions and the ligands, the wide range of coordination numbers, geometry, ligand versatility, capacity for ligand exchange, and redox activity may open up a wide range of design options for therapeutic agents that are not possible with purely organic compounds [9].

Copper, the third most-abundant transition bio-metal, is a key structural component in a number of enzymes and plays a crucial role in all living species [5,12]. Over the years, the coordination chemistry of copper has received huge attention due to its biological, catalytic, redox, and photophysical properties [12,13]. Moreover, copper complexes

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